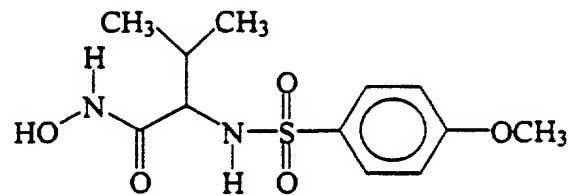
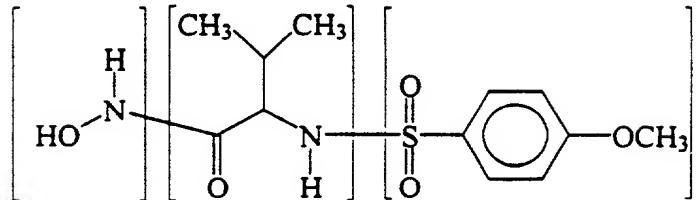


Compound CI



C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub>S



Molecular formula      F<sub>i</sub>      F<sub>ii</sub>      F<sub>iii</sub>

H<sub>2</sub>NO      C<sub>5</sub>H<sub>9</sub>NO      C<sub>7</sub>H<sub>7</sub>O<sub>3</sub>S

Figure 1

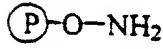
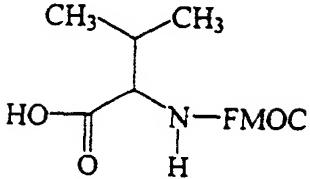
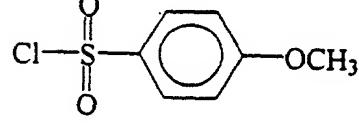
Addition of fragments to yield compounds

Table

Fragment Identifier	Structure	Name	Molecular formula	Other
F <sub>i</sub>		Hydroxylamine	H <sub>2</sub> NO	...
F <sub>ii</sub>		Amino acid	C <sub>5</sub> H <sub>9</sub> NO	...
F <sub>iii</sub>		Sulfonyl	C <sub>7</sub> H <sub>7</sub> O <sub>3</sub> S	...

09753669 "C44LEP3"

Figure 2

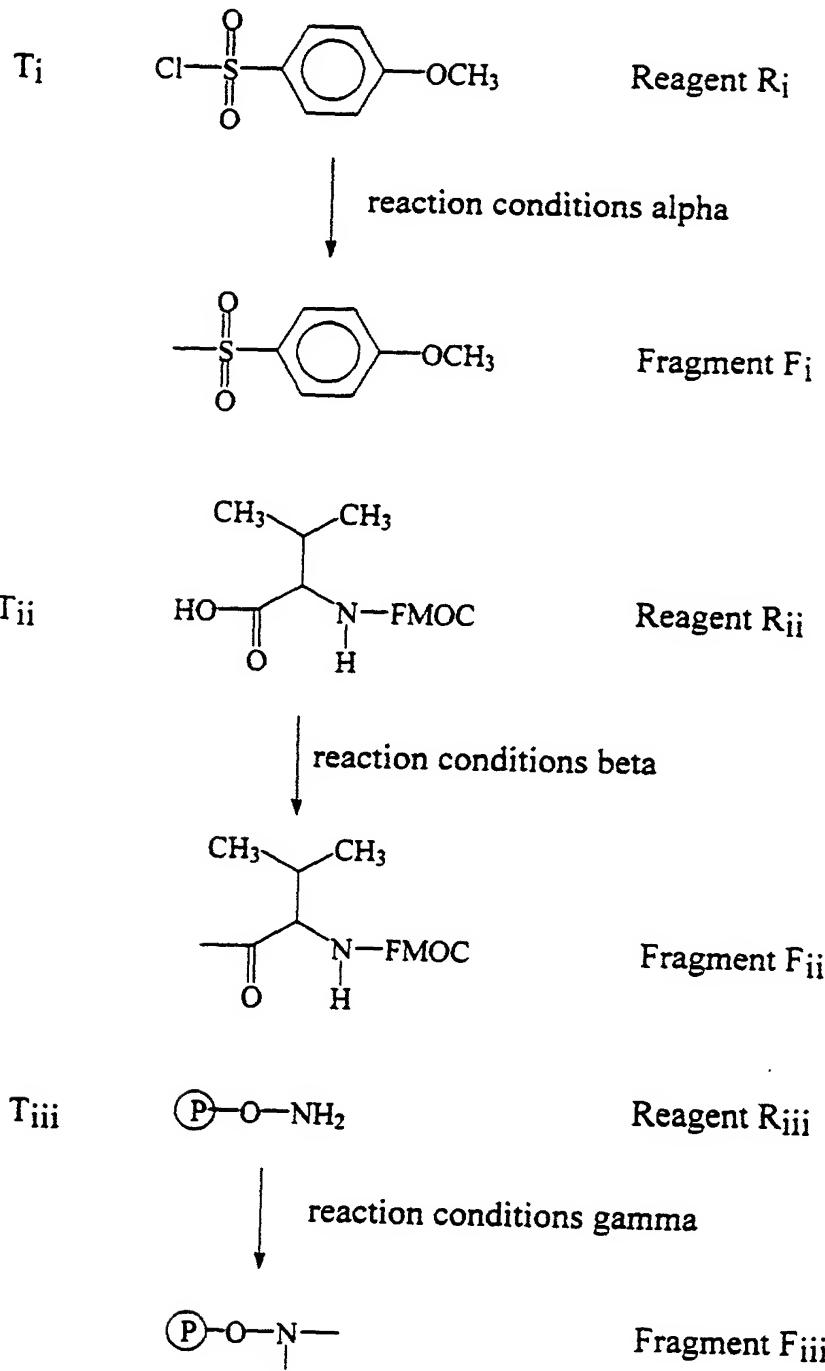
Reagents	Identifier	Name	Properties
H—O—NH <sub>2</sub> or 	R <sub>i</sub>	Hydroxylamine	...
	R <sub>ii</sub>	FMOC blocked amino acid	...
	R <sub>iii</sub>	Sulfonylchloride	...

 = Solid support

09253259-042604

Figure 3

Transformation



(P) = Solid support

Figure 4

Common Fragment / Different Reagents and Transformations

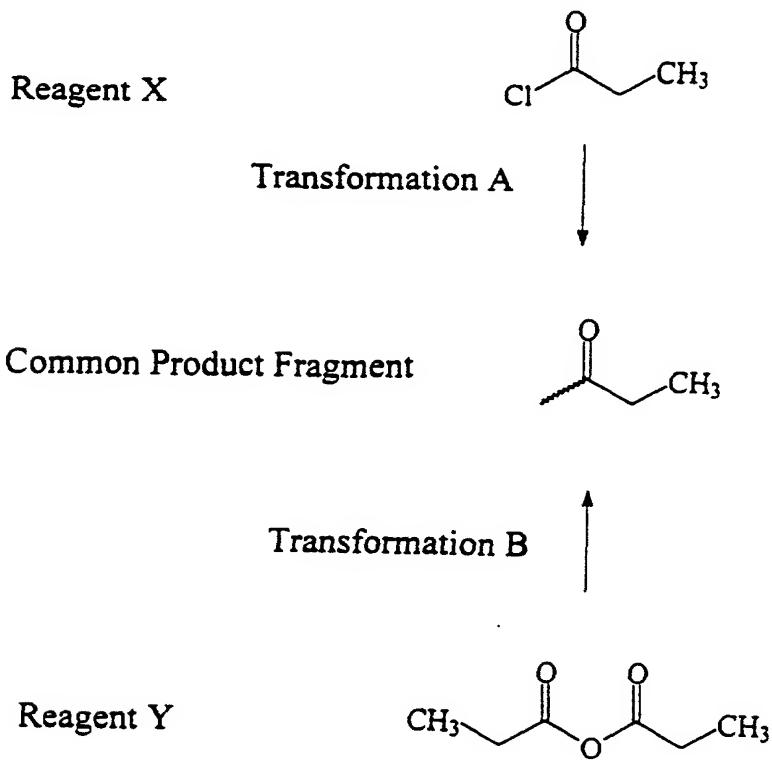


Figure 5

## Common Fragment / Different Reagents and Transformations

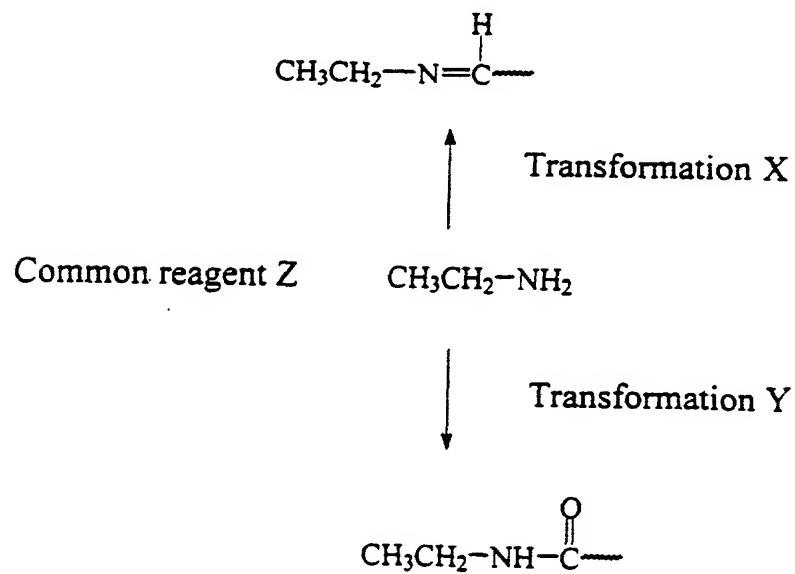
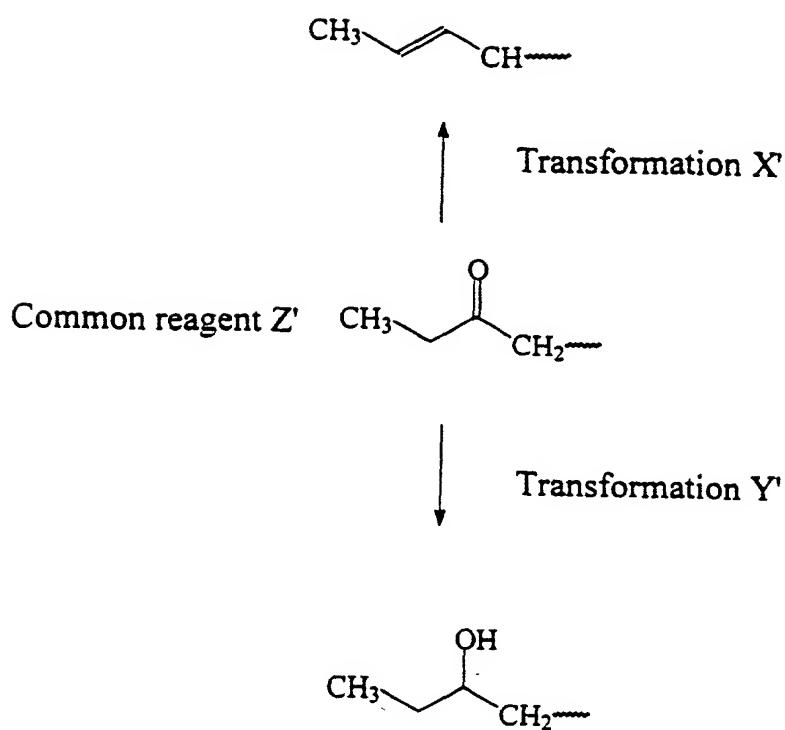


Figure 6a

REAGENTS AND TRANSFORMATIONS

Common Reagent



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Figure 6b

Symbolic addition of fragments to yield compound

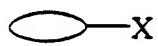
<u>Symbolic Structure</u>	<u>Symbolic Identifier</u>	<u>Molecular formula</u>
---------------------------	----------------------------	--------------------------

Fragment



F<sub>i'</sub>

C<sub>u</sub>H<sub>v</sub>N<sub>w</sub> ...



F<sub>ii'</sub>

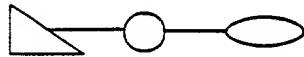
C<sub>u</sub>H<sub>v</sub>N<sub>w</sub> ...



F<sub>iii'</sub>

C<sub>u</sub>H<sub>v</sub>N<sub>w</sub> ...

Compound



C<sub>l'</sub>

C<sub>u</sub>H<sub>v</sub>N<sub>w</sub> ...

Molecular formula F<sub>i'</sub>

+

Molecular formula F<sub>ii'</sub>

+

Molecular formula F<sub>iii'</sub>

= Molecular formula C<sub>l'</sub>

Figure 7

Symbolic Reagent Table

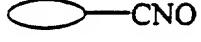
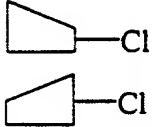
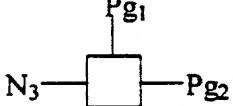
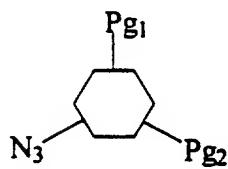
<u>Identifier</u>	<u>Name</u>	<u>Structure</u>	<u>Molecular formula</u>
R1	xxx		xxx
R2	...		...
R3	...		...
R4	...		...
R5	...		...
R6	...		...
R7	...		...
R8	...		...
R9	...		...
R10	...		...

Figure 8

### Symbolic Fragment Table

<u>Identifier</u>	<u>Symbolic Structure</u>	<u>Molecular formula</u>	<u>Molecular Weight</u>
F1		xxx	xxx
F2		...	...
F3		...	...
F4		...	...
F5		...	...
F6		...	...
F7		...	...
F8		...	...

Figure 9

### Symbolic Transformation Table

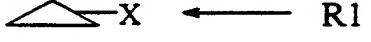
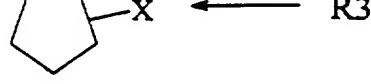
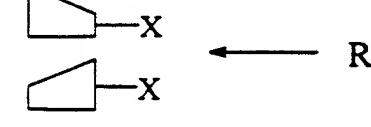
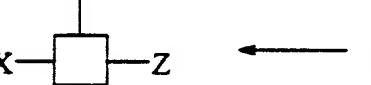
<u>Identifier</u>		<u>Symbolic Reactions</u>	<u>Reagent</u>
T1	F1		conditions $\alpha$
T2	F2		conditions $\beta$
T3	F3		conditions $\alpha$
T4	F3		conditions $\alpha$
T5	F4		conditions $\alpha$
T6	F5		conditions $\varepsilon$
T7	F5		conditions $\alpha$
T8	F6		conditions $\alpha$
T9	F7		conditions $\gamma$
T10	F8		conditions $\gamma$

Figure 10

### Single Compounds and Mixtures

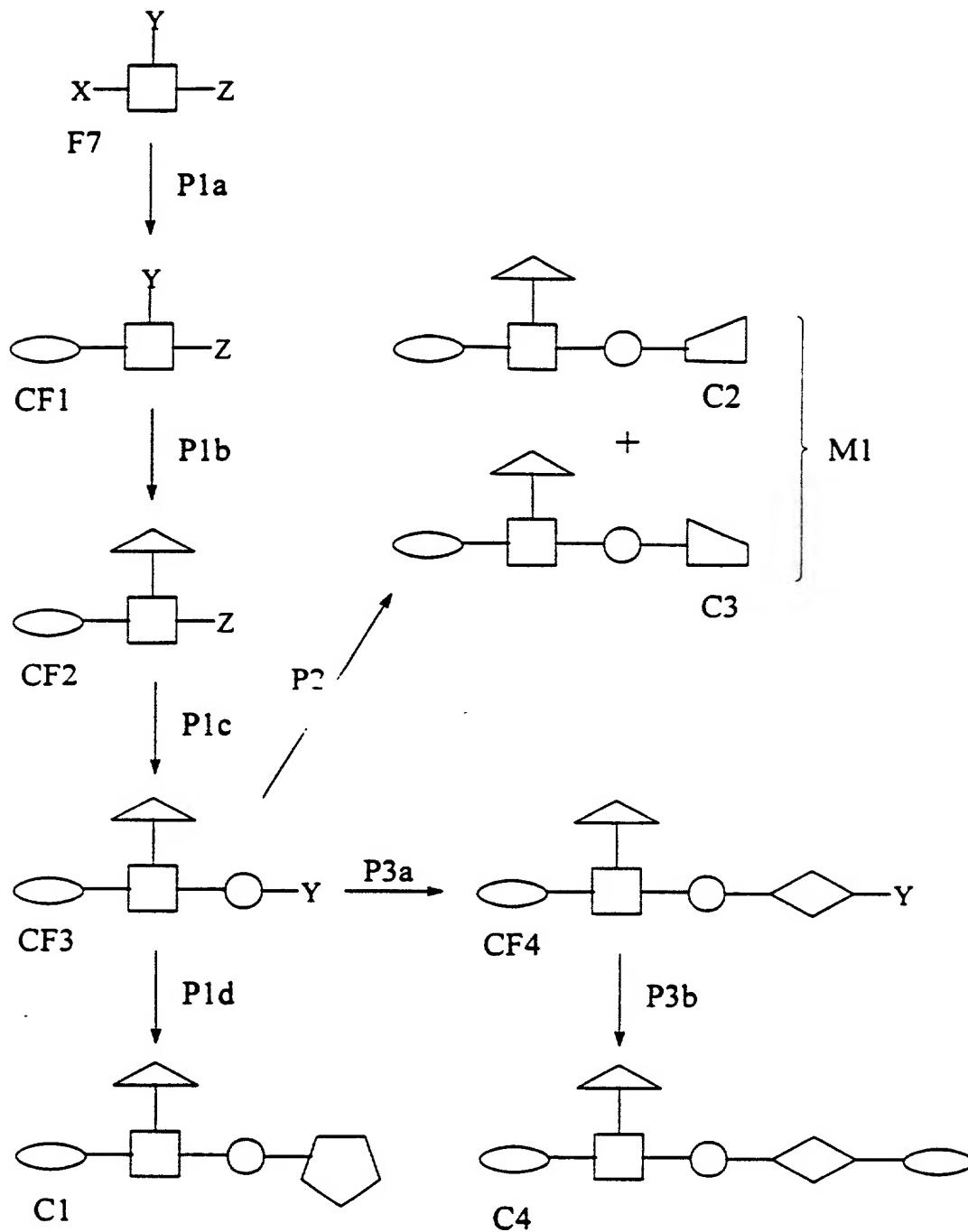


Figure 11

Sheet 13 of 20  
**Mixture 2**

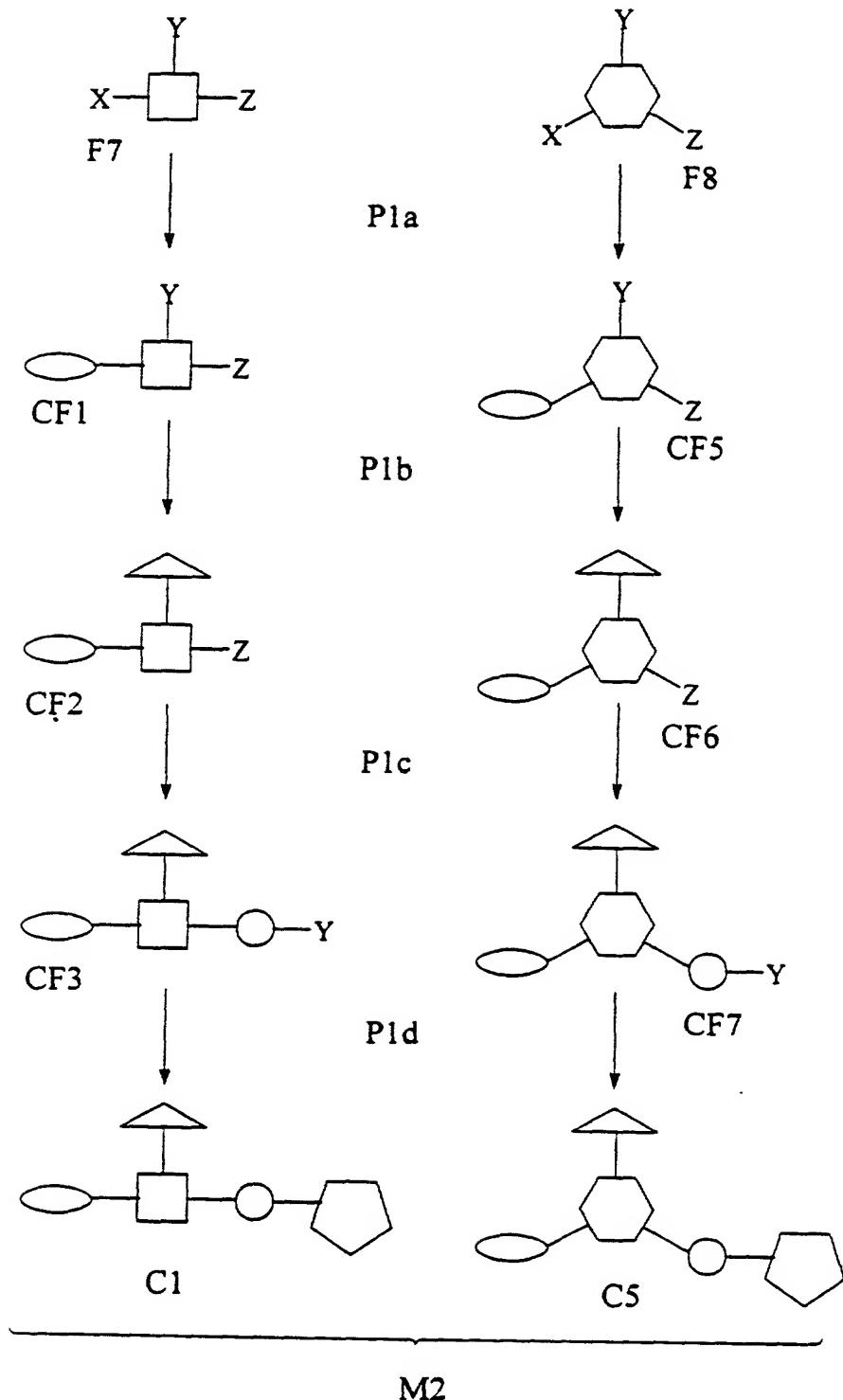


Figure 12

Mixture 3

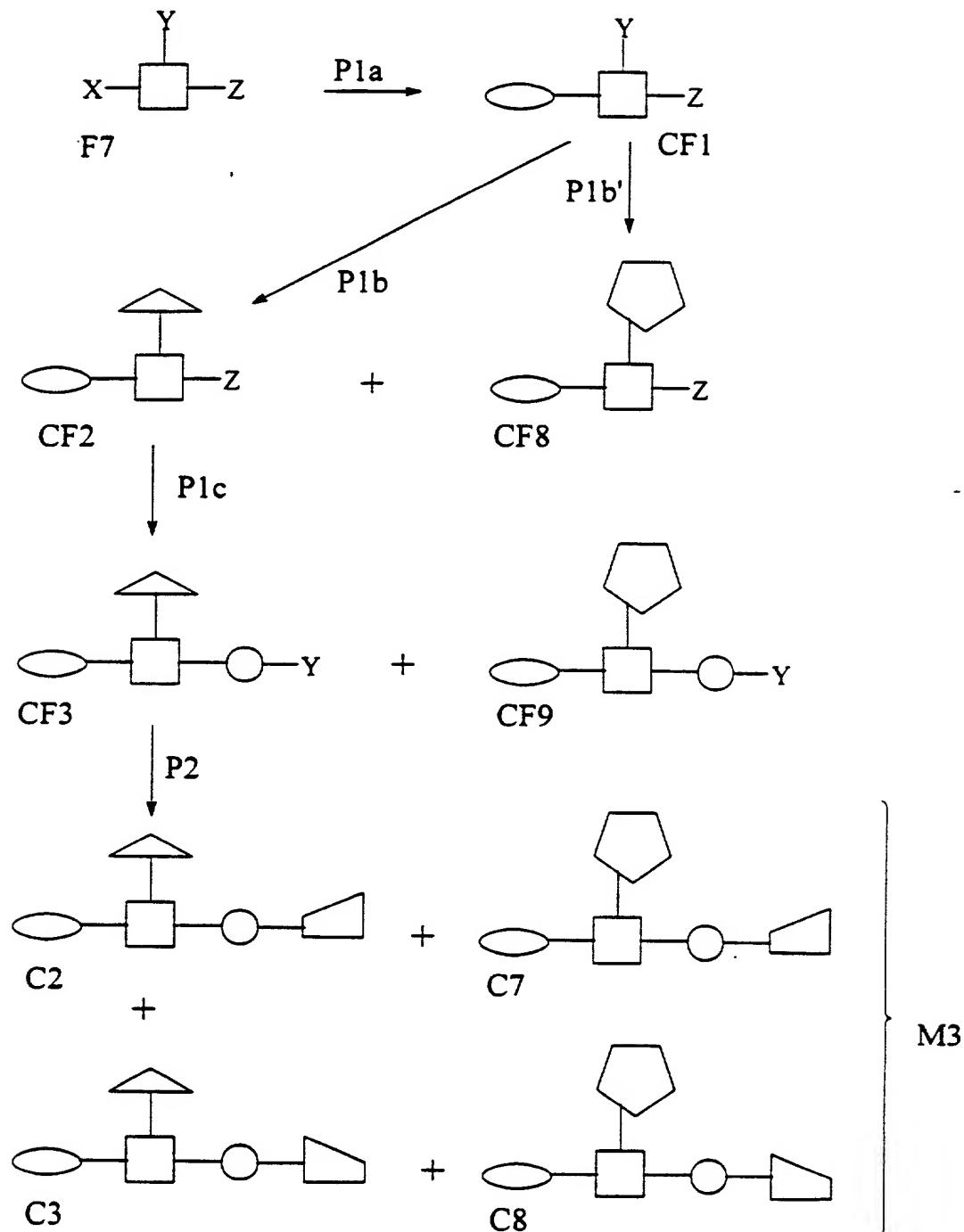
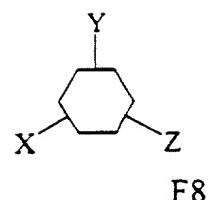
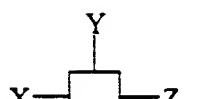


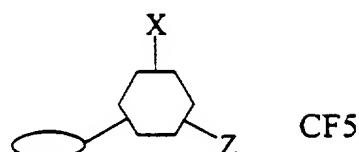
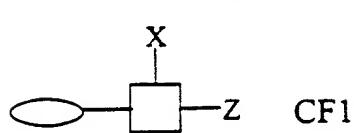
Figure 13

Mixture 4

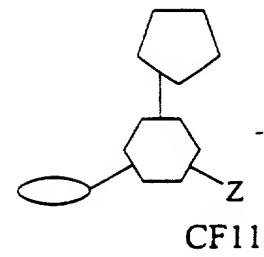
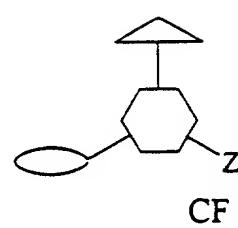
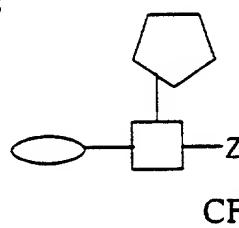
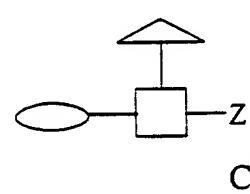
2 Starting Fragments



2 Complex Fragments



4 Complex Fragments



8 Complex Fragments

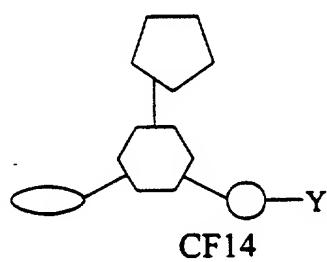
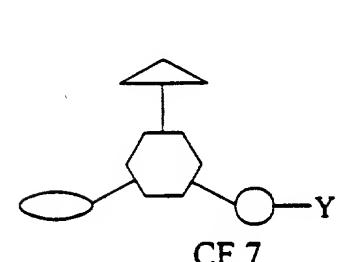
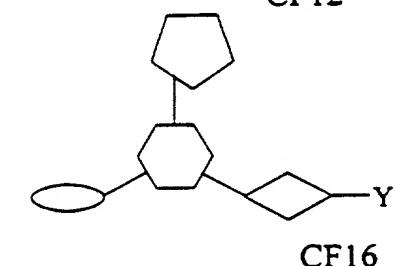
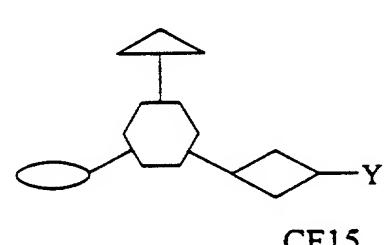
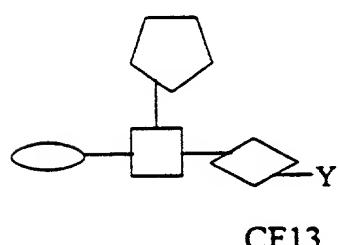
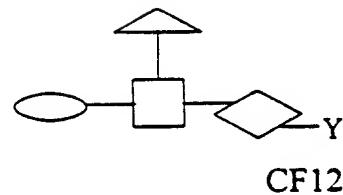
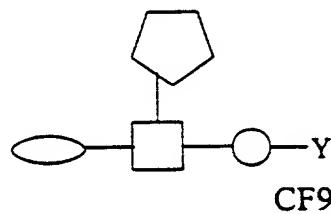
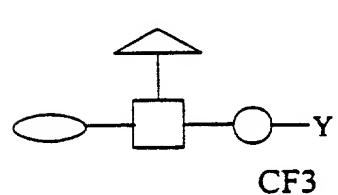


Figure 14a

Mixture 4 (continued)

16 compounds

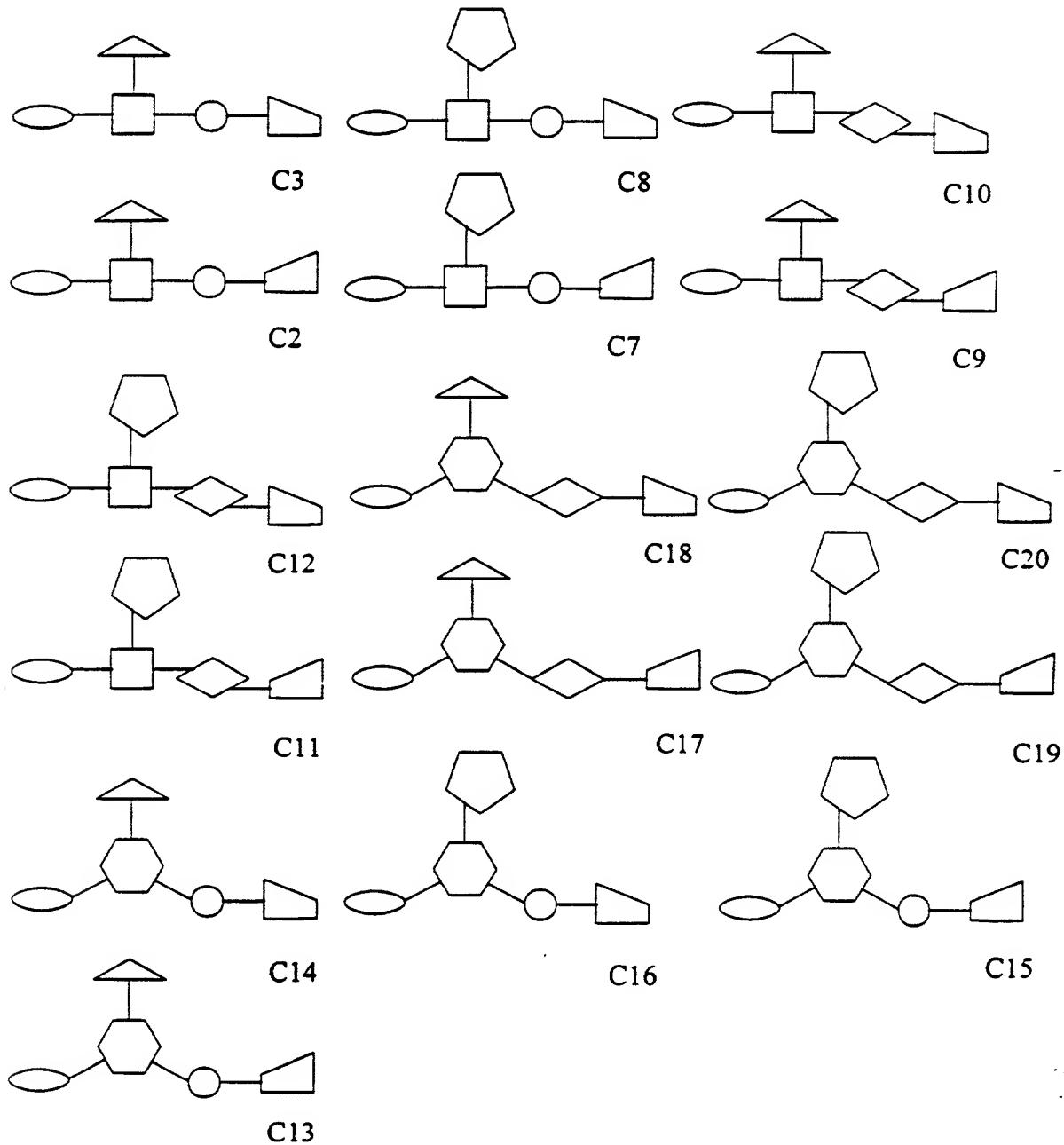


Figure 14b

Tracking Table for Compound C1

(a) By Fragments:

<u>n</u>	<u>n+1</u>	<u>n+2</u>
F7		
	F2	
	F1	
	F5	
		F3

(b) By Transformations:

Synthesis Path 1

<u>n</u>	<u>n+1</u>	<u>n+2</u>
T9		
	T2	
	T1	
	T6	
		T3

Synthesis Path 2

<u>n</u>	<u>n+1</u>	<u>n+2</u>
T9		
	T2	
	T1	
	T7	
		T3

Synthesis Path 3

<u>n</u>	<u>n+1</u>	<u>n+2</u>
T9		
	T2	
	T1	
	T6	
		T4

Synthesis Path 4

<u>n</u>	<u>n+1</u>	<u>n+2</u>
T9		
	T2	
	T1	
	T7	
		T4

Figure 15

Tracking Table

Tracking M1

Step 1		
T9		

Step 2		
T9	T2	

Step 3		
T9	T2 T1	

Step 4		
T9	T2 T1 T7	

Step 5		
T9	T2 T1 T7	T5 <sup>1</sup>

C2

Step 5		
T9	T2 T1 T7	T5 <sup>2</sup>

C3

Figure 16

Sheet 19 of 20

Tracking Table

Tracking M2

Step 1		
n	n+1	n+2
T9		

Step 1		
n	n+1	n+2
T10		

Step 2		
n	n+1	n+2
T9	T2	

Step 2		
n	n+1	n+2
T10	T2	

Step 3		
n	n+1	n+2
T9	T2 T1	

Step 3		
n	n+1	n+2
T10	T2 T1	

Step 4		
n	n+1	n+2
T9	T2 T1 T7	

Step 4		
n	n+1	n+2
T10	T2 T1 T7	

Step 5		
n	n+1	n+2
T9	T2 T1 T7	T4

Step 5		
n	n+1	n+2
T10	T2 T1 T7	T4

C1

C5

Figure 17

Tracking Table

Tracking M3

Step 1

T9	
----	--

Step 2

T9	T2
----	----

Step 3

T9	T2	
	T1	

Step 3

T9	T2	
	T3	

Step 4

T9	T2	
	T1	
	T7	

Step 4

T9	T2	
	T3	
	T7	

Step 5

T9	T2	
	T1	
	T7	
	T5 <sup>1</sup>	

C2

Step 5

T9	T2	
	T1	
	T7	
	T5 <sup>2</sup>	

C3

Step 5

T9	T2	
	T3	
	T7	
	T5 <sup>1</sup>	

C7

Step 5

T9	T2	
	T3	
	T7	
	T5 <sup>1</sup>	

C8

Figure 18